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Modeling of TCE in Adipose Tissue:
Triehloroethylenc (TCE) is a solvent that has been widely used in government (e.g.,USAF) and industrial projects as a metal-decreasing agent, and is now a common soil and groundwater contaminant. Numerous studies have linked TCE and several of its metabolites to short-term toxic health effects such as headaches, dizziness and drowsiness, as well as long—term effects including kidney, liver and lung tumors (see [1]).TCE is highly soluble in lipids, and is known to accumulate in the adipose (fat) tissue of humans and animals. This important characteristic of TCE has major implications on its dynamics inside the organs and tissues, and on the overall amount of time it takes for TCE to be eliminated from the body. Physiologically based pharmacokinetic (PBPK) models are used in the field of toxicology to describe the systemic transport behavior of compounds such as TCE.

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Dynamic Modeling and Control in PBPK Models for Toxic Agents
Electromagnetic Imaging and Active Stealth

AFOSR F49620-01-1-0026

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Final Technical Report
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Objectives

This project had three major objectives: (i) the development of an inverse problem methodology (theoretical, statistical and computational) for parameter estimation in the presence of (model and data) uncertainty. Applications investigated include tissue dissipation of electromagnetic pulsed waves and molecular based models for polymers; (ii) the development of electromagnetic interrogation and anti-interrogation ("active stealth") methodologies. This includes research on use of moving acoustic interfaces as virtual "mirrors" to reflect electromagnetic interrogation signals, development of polarization models to characterize complex composite materials, and development of stealth methodologies in an electromagnetic pursuit/evasion (two player, min-max game theoretic) framework. and (iii) development of molecular based models for hysteresis in polymers and models for electromagnetic/polymeric interactions.

Summary of Accomplishments:

1. *Modeling of TCE in Adipose Tissue:*

Trichloroethylene (TCE) is a solvent that has been widely used in government (e.g., USAF) and industrial projects as a metal-degreasing agent, and is now a common soil and groundwater contaminant. Numerous studies have linked TCE and several of its metabolites to short-term toxic health effects such as headaches, dizziness and drowsiness, as well as long-term effects including kidney, liver and lung tumors (see [1]). TCE is highly soluble in lipids, and is known to accumulate in the adipose (fat) tissue of humans and animals. This important characteristic of TCE has major implications on its dynamics inside the organs and tissues, and on the overall amount of time it takes for TCE to be eliminated from the body.

Physiologically based pharmacokinetic (PBPK) models are used in the field of toxicology to describe the systemic transport behavior of compounds such as TCE. These compartmental models are useful in determining the effective dosage level received by each of the organs and tissue, and are part of the overall process of determining a compound's toxicity to humans and animals. PBPK models usually involve a system of coupled algebraic and differential equations, where each equation represents the transport of the compound through a given organ or tissue. The standard compartmental equations are based on assumptions of rapid equilibrium and uniformity in concentrations within that particular tissue.

These "well-mixed"' assumptions may not be appropriate for highly lipophilic chemicals such as TCE inside the adipose tissue, as several studies have demonstrated large degrees of physiological heterogeneities in fat tissue (see [1]). These heterogeneities include wide variations in fat cell size, lipid distribution, blood flow rates and cell membrane permeabilities. Together, these properties suggest that TCE and other lipophilic compounds are likely to have spatially varying concentrations in the adipose tissue, which further suggests that a spatially varying model may be appropriate for the transport of TCE in the fat.

To test this hypothesis, we have developed three PBPK models for the systemic transport of TCE, where each model has a different submodel for the adipose tissue compartment. The first two adipose compartmental models are based on the standard "well-mixed" assumptions used in PBPK modeling. The third systemic model is a PBPK-hybrid model, with a high-fidelity adipose compartmental model. This spatially varying submodel is based specifically on the physiology of adipose tissue and the expected transport of TCE within the tissue, and utilizes an axial-dispersion type model. See [1] for detailed descriptions of these models.

The TCE PBPK-hybrid model includes a complex coupled system of partial and ordinary differential equations, and it is not immediately evident that solutions for this system of equations in fact exist. In [4,5] we developed theoretical results that guarantee the existence of a unique solution for the TCE PBPK-hybrid model, and we established the convergence of the numerical approximation scheme that we implemented computationally to generate model simulations.

This numerical approximation scheme and the resulting model predictions are presented in detail in [3,5]. A comparison of simulations for the three models demonstrates that the PBPK-hybrid model with the dispersion-based adipose compartment is best able to predict the expected behavior of TCE inside the adipose tissue.

The TCE PBPK-hybrid model is dependent on many physical, biological and chemical parameters, some of which can be explicitly measured. However, most of the adipose model parameters are unknown, and it would be impractical to measure them experimentally. Therefore, inverse problem techniques must be utilized to estimate these model parameters. In [2,5] we developed and implemented several parameter estimation methods for the TCE PBPK-hybrid model with simulated data. Moreover, we addressed issues of uncertainty that arise in the type of experimental data used in toxicokinetics. Specifically, we generated simulated data that approximate the type of variability in parameter values that occurs across a population of individuals, and we developed probability-based estimation methods to account for and incorporate this variability into the parameter estimation process. The results in [2,5] strongly suggest that these probability-based methods are well-suited for parameter estimation problems that involve such variability in the model parameters.

2. *Damage Detection Using Eddy Current Techniques:*
An early focus of our efforts involves the use of ECT (eddy current techniques) [10] to detect subsurface damage (cracks, disbonds, etc.) in structures. We considered a model associated with a specific eddy current method. Making some simplifying assumptions we reduced the three-dimensional problem to a two-dimensional problem for proof-of concept. We then explored theoretical issues relating to the well-posedness of the associated model, establishing the existence and uniqueness of solutions of the variational form and continuous dependence of the solution on parameters describing the damage. We also investigated theoretical issues related to the least squares parameter estimation problem.

To solve the identification problem numerically, an optimization algorithm is employed

which requires solving the forward problem numerous times. To implement these methods in a practical setting, the forward algorithm must be solved with extremely fast and accurate solution methods. Therefore in constructing these computational methods, we employed reduced order Karhunen-Loeve (also called PCA or POD) techniques which allow one to create a set of basis elements spanning a data set consisting of either numerical simulations or experimental data. We investigated two different approaches to forming the reduced order POD approximation of a solution, using a standard Galerkin approach and using interpolation techniques. In general, the POD/Interpolation technique provided a much better approximation [11, 12, 13, 14]

We then [24] tested the proposed methodology on both simulated data as well as experimental data obtained from a GMR sensor in which we tried to estimate parameters describing the geometry of the damage. Using simulated data with 10% relative error, we achieved extremely accurate results. Moreover, we were able to use less than 10 POD basis elements to approximate a finite element solution requiring over 7000 basis elements. This led to a decrease in overall computational time by a factor of 103 for the inverse problem. Applying this methodology to experimental data, we again achieved extremely accurate results. Furthermore, we were able to successfully use experimental data in the formation of the POD basis elements. This illustrates the effectiveness of this method on a wide range of applications. Taken as a whole, our work on this project indicates that using a POD based computational methodology NDE research can be an attractive alternative to the standard finite element methods, offering the potential for substantial savings in total computational time and suggesting feasibility of hand-held, real-time interrogation devices. This basic research has provided a foundation for computational efforts at NASA LaRC in the area of nondestructive evaluation of structures (see Transitions below).

3. *Electromagnetic Interrogation of Dielectric Materials:*
Significant progress has been achieved in several areas in our efforts on use of electromagnetic signals to interrogate materials. In collaborative efforts with the group led by Dr. R.A. Albanese, AFRL, Brooks AFB, we have developed computational methods for the inverse problems of using both conductive interfaces and acoustic wavefronts as reflectors to promote microwave pulse interrogation of materials for both dielectric properties and geometry. The details of the initial work appeared in a monograph [6] published by SIAM. Specifically, in [6] we describe models and applications for techniques which employ superconductive metal backings and *standing* acoustic waves as reflectors for the electromagnetic waves. In addition, we propose a technique in which a *traveling* acoustic wave is used as a virtual interface to reflect an oncoming electromagnetic wave. Analysis of this technique has been the focus of our recent work.

As a first step in assessing this interrogation technique, we considered the equations describing an acoustic pressure wave produced by a windowed sine wave pulse traveling through a layered medium and developed computational methods for solving these equations. Our approximation methods, which result in large algebraic systems, and our computational findings are explained and presented in [7,8].

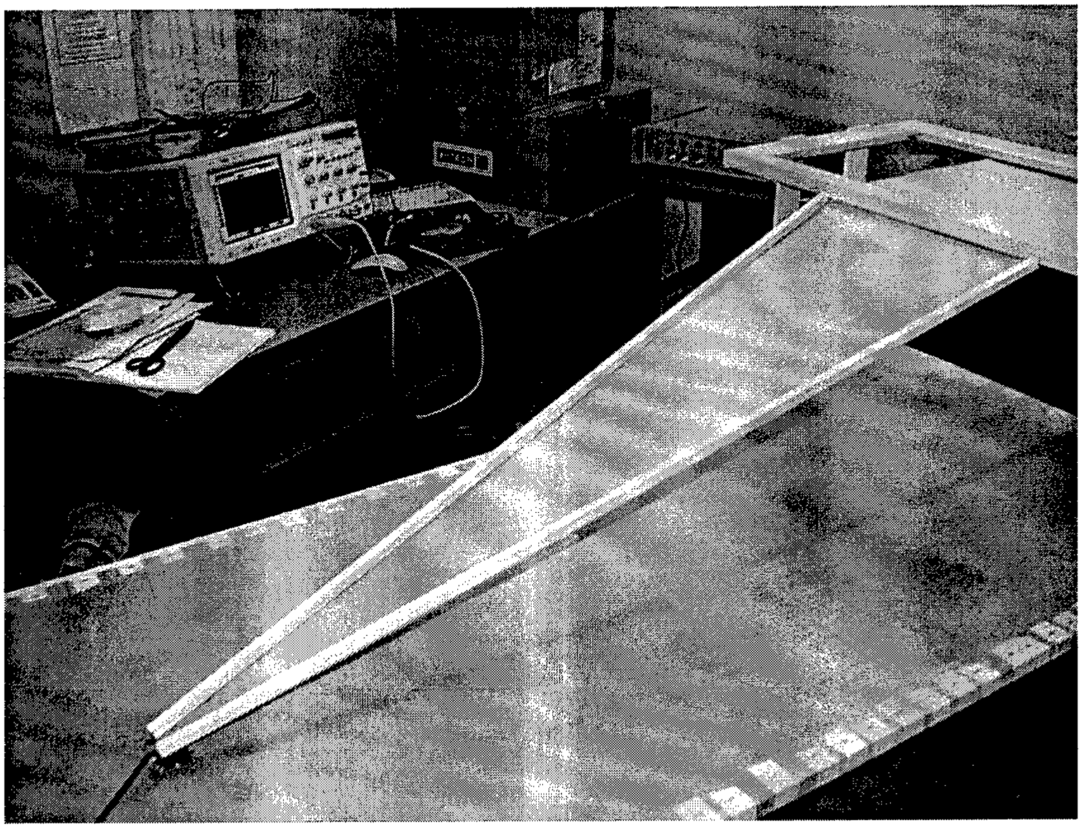

Figure 1. CRSC experimental antenna

A critical second step was to develop a model to describe the electromagnetic/acoustic interaction that results in the reflection of the electromagnetic wave. We began by considering two standard polarization models, those of Debye and Lorentz. Each of these models consists of an ordinary differential equation with constant coefficients. We investigated the possibility that these coefficients are pressure-dependent as a mechanism for acoustic/electromagnetic interaction. Thus, we let each be a linear function of the pressure in the dielectric material. For example, the relaxation parameter τ which is present in both models, becomes

$$\tau = \tau(p) = \tau_0 + K_\tau p$$

where $p = p(t, z)$ is the acoustic pressure in the dielectric. The models are described in detail in [9].

Once the models were developed, they were coupled with Maxwell's equations to describe the proposed interaction between the electromagnetic and acoustic waves. This interaction, however, is best understood by analyzing the systems both theoretically and computationally. We have constructed and implemented approximation schemes to numerically solve the system corresponding to the Debye polarization model. These approximate solutions show the desired interaction between the two waves [9]. In

addition, we have solved the resulting inverse problem and have been able to accurately estimate the polarization coefficients, even in the presence of noise. We have also pursued similar results for the Lorentz system. A second focus of our work entails two and three dimensional versions of the problems, theory and computation developed in [6]. Theoretical and computational results for two dimensional oblique incident interrogation problems have been developed using fixed interfaces (air/dielectric, metallic backing, etc.) as reflectors [45, 47]. A combination of PMLs and absorbing boundary conditions are used to minimize reflections from finite computational boundaries in exploration of both finite element and finite difference schemes [33, 66]. Reduced order computational schemes [39] have proven effective in fixed reflecting surface problems. Theory and computational methods have been developed for problems involving moving acoustic wave fronts (virtual interfaces) reflecting surfaces [9, 30, 66]. An experimental effort to validate the efficacy of using electromagnetic/acoustic interactions in interrogation schemes has begun. Several antennas have been constructed (Figure 1) and we are in the initial stages of collecting data as we refine experimental protocols. These efforts are in close collaboration with Dr. R.A. Albanese (AFRL, Brooks AFB) and his associates.

Initial results for a stealth capability against the electromagnetic interrogations utilizing controllable dielectric layers in the subskin of a conducting object have been obtained [67]. An example problem was formulated in the context of a differential game and/or a robust optimization problem. The scattered field due to interrogations is attenuated assuming an uncertainty in the interrogation wave numbers. A controllable sublayer composed of ferromagnetic and ferroelectric materials is incorporated in the mathematical formulation based on the time-harmonic Maxwell equation. Fresnel's law for the reflectance index is extended to electromagnetic propagation in anisotropic composite layers of ferro-magnetic and ferro-electric devices. The methodology has been successfully tested for non-planar 2D geometry of a conducting object with particular findings for a standard NACA airfoil.

Finally, our efforts [33, 46] on high frequency (Terahertz) full wave nonlinear methods for the above problems have begun in collaboration with G. Pinter (U. Wisconsin, Milwaukee). We have investigated linear verses nonlinear Debye polarization in materials to date.

4. *Inverse Problem Methodology:* We have made excellent progress in efforts on an inverse problem methodology for problems with uncertainty (variability) in both the model dynamics and data. A general theoretical and computational framework has been developed and tested. This framework, based on the Prohorov metric for spaces of probability distributions, has been used with PBPK models for TCE [2, 40, 48] as well as in molecular models for HIV infections [22, 28, 40]. Recent computational efforts [48] to compare the Prohorov metric framework (PMF) to popular Bayesian-based Markov Chain Monte Carlo (MCMC) methods reveal that the PMF methods compare quite famrably on PBPK model problems.

The PMF has also been used in our development of molecular based reptation (internal dynamics) models for hysteresis in polymers such as rubber [62] and tissue [65]. These multi-scale efforts provide a molecular (micro) level model with uncertainty as foundation for systemic (macro) level hysteresis as embodied in general integro-partial

differential equations. Rubber data from experiments (uniaxial tension and shear) have been used with the inverse problem methodology to validate both the approach and the models.

Efforts to understand hysteresis in viscoelastic materials has lead to an extension of the linear "stick-slip" models of Doi-Edwards and Jonson-Stacer to nonlinear reptation models [61, 62]. It is then shown that such models, when combined with probabilistic formulations allowing distributions of relaxation times, provide a good description of dynamic experiments with highly filled rubber in tensile deformations. A connection to other applications including dielectric polarization [64] and reptation in other viscoelastic materials (e.g., living tissue) [32, 65] is now clear and initial computational results based on these ideas for dielectrics is promising. Extensions to include intra-molecular variability in polymers have been made [68].

Personnel Supported

Faculty: H.T. Banks, K. Ito, N.G. Medhin
Post docs and Research Associates: J. Bardsley, V.A. Bokil, B. Browning, , K. Furati, G.M Kepler, J.A. Toivanen, S. Wynne
Graduate Students: B. Benedict, D.M. Bortz, S J. Davis, N.L. Gibson, S. Grove, J.B. Hood, S. Lawler/Ernstberger, N. Luke, L.K. Potter, J.K. Raye, C.J. Smith, L. Stroud/Dick

Transitions:

- Inverse problem methodology in the presence of uncertainty: This work is in collaboration with scientists at GSK (contact: Laura K. Potter, Tel: 919-662-9957, Home) and with scientists at AFRL led by Dr. R.A. Albanese (Tel 210-536-5710). These techniques have direct relevance to emerging efforts on bioterrorism, electromagnetic interrogation in complex materials, and molecular based modeling of polymers.
- Electromagnetic interrogation of dispersive media: Problem formulation and method development involves close collaboration with Dr. Richard Albanese (Tel: 210-536-5710) and colleagues at AFRL, Brooks AFB. The moving acoustic interface reflection problems mentioned above have direct application to Albanese led efforts on material detection and interrogation of interest to AF and DoD (location of subsurface mines, bunkers, characterization of weapons systems stealth technology). The resulting technology will also be directly relevant to stealth technology and detection of hidden toxic agents as well as determination of threat levels in individuals.
- Eddy Current NDE: The project using eddy current techniques in subsurface damage detection is in collaboration with Dr. William Winfree (tel:(757-864-4963) and colleagues at NASA Langley Research Center, Hampton, V A. The methods developed to date are being used in experimental efforts at NASA Langley in our efforts with this group.

Cumulative Honors and Awards:

Banks, AFOSR Research Achievement, 1990, 1996.
Banks, IEEE Fellow, 1994.
Banks, 1995-96 NCSU Alumni Association Outstanding Research Award.
Banks, (with R.C. Smith and R. Silcox).1995 ASME Adaptive Structures "Best Paper Award in Structural Dynamics and Control"; presented at the 1996 Adaptive Structures Forum, Salt Lake City, Utah, April, 1996.
Banks, IEEE-CSS Control Systems Technology Award, Kobe, Japan, Dec. 1996.
Banks, Distinguished Alumnus Award, Purdue University, 1998.
Banks, SIAM Board of Trustees, Jan.,1997-Dec, 2002; Elected Chairman, SIAM Board of Trustees, 1999, re-elected, 2000; re-elected, 2001; re-elected, 2002.
Banks, Institute of Physics Fellow, 1999.
Banks, Alumni Distinguished Graduate Professor, NCSU, 2000.
Banks, (with G.A. Pinter and O.H. Yeoh), Best Paper Award, Rubber Division of American Chemical Society, Cincinnati, OH, Oct. 2000.
Banks, W.T. & Idalia Reid Prize in Applied Mathematics, SIAM 50th Anniversary Meeting, Philadelphia, PA, July 9, 2002.
Banks, Elected Chair, SIAM Activity Group on Control, August, 2002.
Banks, Turkish Governors Award for "Outstanding Contributions to Inverse Problems", Fethiye, Turkey, June 6, 2004.
B.M. Adams, GAANN Fellow, 2000-2003.
B. Benedict, NASA Fellow, 2003-2006.
D.M. Bortz, GAANN Fellow, DOE, 1998-2001.
N.L. Gibson, NASA Fellow, 2002-2004.
N. Luke, David and Lucile Packard Fellow, 2001-2006.
J. Davis, DOE Comp. Sci. Fellow, 2004-2008.
S. Lawler/Ernstberger, DHS Fellow, 2004-2008.
L.K. Potter, NSF Graduate Fellow, 1996-2000.
J.K. Raye, GAANN Fellow, DOE, 1996-2000.
C.J. Smith, Lord/CRSC Fellow, 2001-2003.

Publications: (supported in part under this grant)

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[7] H.T. Banks and J. K. Raye, "Computational methods for nonsmooth acoustic systems", Technical Report CRSC-TR01-02, Center for Research in Scientific Computation, North Carolina State University, Raleigh, NC, 2001.

[8] H.T. Banks and J. K. Raye, "Computational methods for nonsmooth acoustic systems arising in an electromagnetic hysteresis identification problem", *Proceedings of the 18th ASME Biennial Conference on Mechanical Vibration and Noise,* Pittsburgh, P A, September 9-12, 2001.

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